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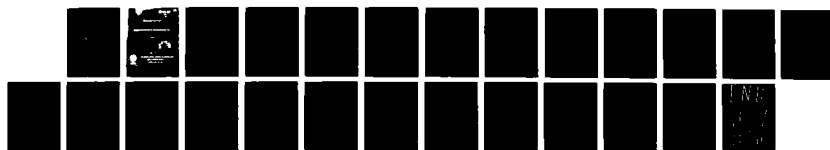
MOLECULAR STRUCTURE OF TRIAMINOGUANIDINE (TAG)(U) ARMY
ARMAMENT RESEARCH DEVELOPMENT AND ENGINEERING CENTER
DOVER NJ ARMAMENT ENGINEERING DIRECTORATE A J BRACUTI
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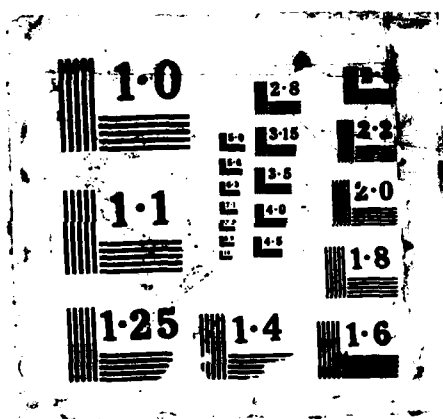
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SECURITY CLASSIFICATION OF THIS PAGE

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INTRODUCTION

The U.S. Army Armament Research, Development and Engineering Center (ARDEC) has successfully isolated the free-base of the triaminoguanidinium ion (ref 1). Subsequent elemental analysis suggested that the solid free base was actually triaminoguanidine (TAG CN_8H_8) rather than triaminoguanidinium hydroxide (TAGOH $\text{CN}_8\text{H}_9\text{O}$). This was also suggested in an earlier investigation (ref 2), but was not verified by experimental evidence. To ascertain the nature of the free-base unequivocally, a molecular structure determination was undertaken.

DISCUSSION

Data Collection

A colorless plate-like crystal of the free base approximately $0.15 \times 0.06 \times 0.30$ mm was mounted on a glass fiber with the longest axis approximately parallel to the ϕ axis of the goniometer. The preliminary examination and data collection were performed with $\text{CuK}\alpha$ radiation ($\lambda = 1.54184$ Å) on the Enraf-Nonius CAD4, computer controlled, kappa axis diffractometer equipped with a graphite crystal incident beam monochromator.

Cell constants and orientation matrix for data collection were obtained from least-squares refinement, using the setting angles of 23 reflections in the range of $9 < \theta < 74$ measured by the computer-controlled diagonal slit method of centering. As a check on crystal quality, omega scans of several intense reflections were measured. The width at reflection intensity half-height was 0.20 degrees with a take-off angle of 5.8, which indicates good crystal quality.

The intensity data were collected at a temperature of $-105 \pm 1^\circ\text{C}$ using the $\omega - \theta$ technique with a scan rate varying from 2 to 25 per min (in omega). The variable scan rate allows rapid data collection of intense reflections and also assures good counting statistics for weak reflections where a slow scan should be used. Intensity data for 1,659 reflections of which 932 were unique and not systematically absent with $h = 0$ to 9, $k = 0$ to 12, and $l = -7$ to 7 were collected to a maximum 2θ value of 150.0. The scan range (in degrees) was determined as a function of θ to correct for the separation of the $\text{K}\alpha$ doublet (ref 3). The scan was calculated by the equation

$$\text{Scan width} = 0.9 + 0.300 \tan \theta$$

All background counts were measured with the moving-crystal moving-counter technique by scanning an additional 25% above and below this range. Thus, the ratio of peak counting time to background counting time was 2:1. The horizontal aperture width ranged from 2.0 to 5.7 mm while the vertical aperture was set at 2.0 mm. The diameter of the incident beam collimator was set at 0.7 mm and the crystal-to-detector distance was 21 cm. For intense reflections an attenuator (attenuation factor of 15.5) was automatically inserted in front of the detector.

As a check on both the crystal and electronic stability, three representative reflections were measured every 41 minutes. The intensities of these standards remained constant within experimental error throughout data collection. No decay correction was applied to these data.

Data Reduction

Lorentz-polarization and secondary extinction corrections (ref 4), but no absorption corrections, were applied to the intensity data. The final extinction coefficient refined in least squares to a value of 0.0000170 (in absolute units). The intensities of equivalent reflections were averaged. The agreement factors for the averaging of the 3,482 observed reflections was 3.7% based on intensity and 2.3% based on F_o .

The crystal data are:

Monoclinic, space group $P2_1/c$ (#14), $a = 7.460(3)$, $b = 10.274(2)$,
 $c = 6.343(3)$ Å, $\beta = 110.80(2)$, $V = 454.5$ Å³, $Z = 4$, $D_x = 1.52$ g/cm³
 $\rho = 10.1/\text{cm}^3$, $F(000) = 224$, $F_w = 104.12$, $T = 168\text{K}$ (-105°C) systematic
 absences: $0k0$, $k = 2n + 1$; $h0l$, $l = 2n + 1$.

On the basis of systematic absences and E probability distribution statistics, the centrosymmetric space group $P2_1/C$ was selected.

Structure Determination

The structure was solved by direct methods (Enraf-Nonius structure Determination Package, ref 3). Using 200 reflections (minimum E of 1.331) and 597 relationships, a total of 16 phase sets were produced. The seven non-hydrogen atoms were located from an E-map prepared from the phase set with the following best probability statistics: absolute figure of merit 1.39, residual 0.26, and psi zero 0.690. The remaining hydrogen atoms were located in successive difference Fourier syntheses. The non-hydrogen atoms were refined anisotropically by full matrix, least-squares in which the function $\Sigma = W(|F_o| - |F_c|)^2$ was minimized and w is defined as $4F_o^2/\sigma^2(F_o)$. The standard deviation of intensities, $\sigma^2(F_o)$, is defined as

$$\sigma^2(F_o^2) = [S^2 (2 + R^2 B) + (\rho F_o^2)^2] / (Lp)^2$$

in which S is the scan rate, C is the total integrated peak count, R is the ratio of the scan time to the background count, Lp is the Lorentz-polarization factor, and the parameter ρ is a factor introduced to downweight intense reflections. In this case, ρ was set to 0.060.

The x-ray scattering factors were taken from Cromer and Waber (ref 5). Anomalous dispersion effects were included in the calculation of structure factors (ref 6) and the values of $\Delta f'$ and $\Delta f''$ were those of Cromer (ref 7). Only reflections with intensities greater than 3.0 times their standard deviations were used in the refinements. The final cycle of refinement included 87 variables and converged (largest parameter shift was 0.62 times its esd) with an unweighted agreement factor of $R = 0.031$

$$R = \Sigma (|F_o| - |F_c|) / \Sigma F_o$$

and a weighted agreement factor of $R_w = 0.052$ in which

$$R_w = \text{SQRT} [\Sigma w (|F_o| - |F_c|)^2 / \Sigma w F_o^2]$$

The standard deviation of an observation unit weight was 1.30. The highest peak in the final difference Fourier had a height of 0.25 e/A with an estimated error based on ΔF of 0.05 (ref 8).

Description of Crystal Structure

The atomic coordinants and thermal parameters of the free base are listed in tables 1 and 2, respectively. The unit cell (fig. 1) contains four TAG molecules. This confirms the contention previously reported (refs 1 and 2) that the free base of the triaminoguanidinium ion is actually triaminoguanidine rather than triaminoguanidinium hydroxide (TAGOH).

The crystal structure consists of sheets of TAG molecules oriented in the direction of the b axis which are held together by van der Waals forces and hydrogen bonding. The closest non-hydrogen bonded intermolecular distance [N(2)---N(5), table 3] is 3.220 (1) Å while the closest hydrogen bonded distance [N(2)---N(3), table 4] is 2.967(1) Å with a hydrogen bond length [H(3)---N(2)] of 2.06(2) Å and bond angle [N(3)--H(3)---N(2)] of 156.(1). In addition, there are three other hydrogen-bonded close-contacts: N(5)--H(6)--N(2) with a length of 3.107(1)Å; N(6)--H(7)--N(1) with a length of 3.017(1) Å; and N(2)--H(5)---N(1) with a length of 3.297(1) Å. The unit cell without hydrogen bonding is shown in figure 2, a stereographic pair of unit cells in figure 3.

Description of the Triaminoguanidine Molecule

The TAG molecule presented (fig. 4) does not display the C_{3h} symmetry typical of the TAG cations previously reported (refs 9 and 10). In this case, the three C--N bonds and bond angles (tables 4 and 5) of the guanidine moiety are not equivalent, as they are in the guanidinium moiety of the triaminoguanidinium ion of TAGN [TAGN mean C--N value of 1.322(6) Å]. Of the three bonds, the C--N distance is significantly shorter with a value of 1.292(1) Å, while the equivalent C--N(3) and C--N(5) distances have significantly longer values of 1.373(1) and 1.381(1) Å, respectively. These values suggest that a double bond is localized at C=N(1) and that C--N(3) and C--N(5) are equivalent single bonds. The respective N--N bond distances for N(1)--N(2), N(3)--N(4) and N(5)--N(6) are 1.451(1), 1.425(1) and 1.432(1) Å, which are indicative of three single, but not necessarily equivalent, N--N bonds.

In the TAG ion, an aromatic-like stabilization results from the double-bond resonance observed among the three equivalent C--N bonds. Also this double-bond resonance restricts free rotation about

each C--N bond and, as a result, constrains the ion to a planar conformation (except for the three pairs of non-planar amino hydrogen atoms). Of course, structure dependent, local-perturbations such as electrostatic forces and hydrogen bonding can cause small distortions to the planar conformation as demonstrated in the structure of TAG5AT (ref 11).

In contrast to the TAG ion, double-bond resonance is apparently lost in the TAG molecule by virtue of the formation of a localized double bond in the guanidine moiety [C=N(1)]. This loss of resonance decreases the stability of the free base and also permits free rotation about the two C--N single bonds. The onset of free rotation relaxes the planarity constraint on the amino nitrogen atoms. Hence, one would expect a conformation where only the guanidine moiety is planar in this molecule.

The weighted least-squares planes data (table 6) do, indeed, indicate that only the non-hydrogen atoms of the guanidine moiety are planar (greatest planat deviation 0.002 Å). The two amino hydrogen atoms are involved in intermolecular bonding, which probably contributes to their deviation from the expected planar conformation in the guanidine moiety. The lack of planarity displayed by the TAG molecule is further verified by the torsion angles presented in table 7.

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Table 1. Atomic positions and estimated standard deviations for the triaminoguanidine molecule

<u>Atom</u>	<u>x</u>	<u>y</u>	<u>z</u>
C	0.2343(1)	0.0361(1)	0.1937(2)
N(1)	0.2102(1)	0.13298(9)	0.0561(1)
N(2)	0.3015(1)	0.11152(10)	-0.1083(1)
N(3)	0.3294(1)	-0.07607(10)	0.1797(2)
N(4)	0.3656(1)	-0.16819(10)	0.3580(2)
N(5)	0.1383(1)	0.04159(10)	0.3629(1)
N(6)	-0.0024(1)	0.12554(9)	0.3318(1)
H(1)	0.273(2)	0.188(1)	-0.195(2)
H(2)	0.236(2)	0.039(2)	-0.199(2)
H(3)	0.433(2)	-0.067(2)	0.129(3)
H(4)	0.351(2)	-0.247(2)	0.295(3)
H(5)	0.478(2)	-0.161(2)	0.448(3)
H(6)	0.141(2)	-0.035(1)	0.409(2)
H(7)	0.042(2)	0.203(1)	0.396(2)
H(8)	-0.56(2)	0.143(1)	0.182(2)

Table 2. Anisotropic and equivalent isotropic temperature factors and their estimated standard deviations

<u>Atom</u>	<u>B₁₁</u>	<u>B₂₂</u>	<u>B₃₃</u>	<u>B₁₂</u>	<u>B₁₃</u>	<u>B₂₃</u>	<u>B_{eq}</u>
C	1.03(3)	1.18(4)	0.67(3)	-0.15(3)	0.26(2)	-0.16(3)	0.92(2)
N(1)	1.43(3)	1.28(3)	0.82(3)	0.05(3)	0.68(2)	0.02(3)	1.10(2)
N(2)	1.55(3)	1.43(3)	0.89(3)	0.06(3)	0.75(2)	0.10(3)	1.20(2)
N(3)	1.44(3)	1.24(3)	1.23(3)	0.24(3)	0.77(2)	0.30(3)	1.23(2)
N(4)	2.15(3)	1.58(3)	1.82(3)	0.52(3)	0.98(3)	0.81(3)	1.17(2)
N(5)	1.46(3)	1.17(3)	0.91(3)	0.10(3)	0.69(2)	0.15(3)	1.11(2)
N(6)	1.38(3)	1.21(3)	1.09(3)	0.06(3)	0.65(2)	-0.05(3)	1.17(2)
H(1)	-	-	-	-	-	-	2.2(3)
H(2)	-	-	-	-	-	-	2.3(3)
H(3)	-	-	-	-	-	-	3.1(4)
H(4)	-	-	-	-	-	-	3.4(4)
H(5)	-	-	-	-	-	-	3.4(4)
H(6)	-	-	-	-	-	-	1.5(3)
H(7)	-	-	-	-	-	-	1.8(3)
H(8)	-	-	-	-	-	-	2.4(4)

Table 3. Details of intermolecular hydrogen bonding between donor (D) and acceptor (A) atoms and their estimated standard deviations

<u>D-H-----A</u> <u>atoms</u>	<u>D-----A</u> <u>A</u>	<u>H----A</u> <u>A</u>	<u>Angle</u> <u>deg</u>
N(2)-H(1)---N(1)	3.297(1)	2.37(2)	175.(1)
N(3)-H(3)---N(2)	2.967(1)	2.06(2)	156.(1)
N(5)-H(6)---N(6)	3.107(1)	2.414(5)	133.(1)
N(6)-N(7)---N(1)	3.017(1)	2.133(15)	167.(1)

Table 4. Bond distances in triaminoguanidine

<u>Bond</u>	<u>Distance, Å</u>
C--N(1)	1.292(1)
C--N(3)	1.373(1)
C--N(5)	1.381(1)
N(1)--N(2)	1.451(1)
N(3)--N(4)	1.452(1)
N(5)--N(6)	1.432(1)
N(3)--H(3)	0.98(2)
N(5)--H(6)	0.86(2)
N(2)--H(1)	0.93(2)
N(2)--H(2)	0.96(2)
N(4)--H(4)	0.98(2)
N(4)--H(5)	0.83(2)
N(6)--H(7)	0.901(15)
N(6)--H(8)	0.91(2)

Table 5. Bond angles and estimated standard deviations

<u>Atoms</u>	<u>Angle (deg)</u>
N(1)-C-N(3)	123.57(9)
N(1)-C-N(5)	119.8(1)
N(3)-C-N(5)	116.65(9)
C-N(1)-N(2)	112.43(9)
C-N(3)-N(4)	117.58(9)
C-N(5)-N(6)	118.14(9)
C-N(3)-H(3)	117.1(1)
C-N(5)-H(6)	113.1(1)
N(4)-H(3)-H(3)	115.1(5)
N(6)-N(5)-H(6)	112.1(1)
N(1)-N(2)-H(1)	103.1(9)
N(1)-N(2)-H(2)	106.3(9)
N(3)-N(4)-H(4)	107.(1)
N(3)-N(4)-H(5)	110.(1)
N(5)-N(6)-H(7)	108.4(9)
N(5)-N(6)-H(8)	107.(1)
H(1)-N(2)-H(2)	110.(1)
H(4)-N(4)-H(5)	109.(2)
H(7)-N(6)-H(8)	105.(1)

Table 6. Best weighted least-squares plane for triaminoguanidine

<u>Atoms</u>	<u>Coordinants</u>			<u>Distance off plane A</u>
	<u>x</u>	<u>y</u>	<u>z</u>	
<u>On-plane</u>				
C	1.3115	0.3712	1.1489	0.000(1)
N(1)	1.4414	1.3642	0.3328	0.002(1)
N(3)	2.0525	-0.7816	1.0658	0.002(1)
N(5)	0.3639	0.4273	2.1517	0.002(1)
<u>Off-plane</u>				
N(2)	2.4934	1.1458	-0.6420	-0.031(1)
N(4)	1.9207	-1.7280	2.1228	-0.173(1)
N(6)	-0.7649	1.2898	1.9671	0.536(1)
H(1)	2.4720	1.9265	-1.1554	-0.017(15)
H(2)	2.2117	0.3984	-1.1805	0.791(15)
H(3)	2.9615	-0.6932	0.7087	-0.434(17)
H(4)	1.9540	-2.5417	1.7503	0.360(20)
H(5)	2.5531	-1.6544	2.6575	-0.960(20)
H(6)	0.1262	-0.3568	2.4280	0.340(14)
H(7)	-0.5810	2.0851	2.3493	-0.143(14)
H(8)	-0.3268	1.4681	1.0800	1.049(17)

Table 7. Torsion angles of triaminoguanidine

<u>Atom 1</u>	<u>Atom 2</u>	<u>Atom 3</u>	<u>Atom 4</u>	<u>Angle (deg)</u>
N(3)	C	N(1)	N(2)	-2.4
N(5)	C	N(1)	N(2)	179.1
N(1)	C	N(3)	N(4)	172.6
N(1)	C	N(3)	H(3)	30.9
N(5)	C	N(3)	N(4)	-8.9
N(5)	C	N(3)	H(3)	-150.6
N(1)	C	N(5)	N(6)	24.0
N(1)	C	N(5)	H(6)	156.7
N(3)	C	N(5)	N(6)	-154.5
N(3)	C	N(5)	H(6)	-21.9
C	N(1)	N(2)	H(1)	179.9
C	N(1)	N(2)	H(2)	64.7
C	N(3)	N(4)	H(4)	142.6
C	N(3)	N(4)	H(5)	-99.4
H(3)	N(3)	N(4)	H(4)	-75.0
H(3)	N(3)	N(4)	H(5)	43.0
C	N(5)	N(6)	H(7)	-93.8
C	N(5)	N(6)	H(8)	18.9
H(6)	N(5)	N(6)	H(7)	133.2
H(6)	N(5)	N(6)	H(8)	-114.1

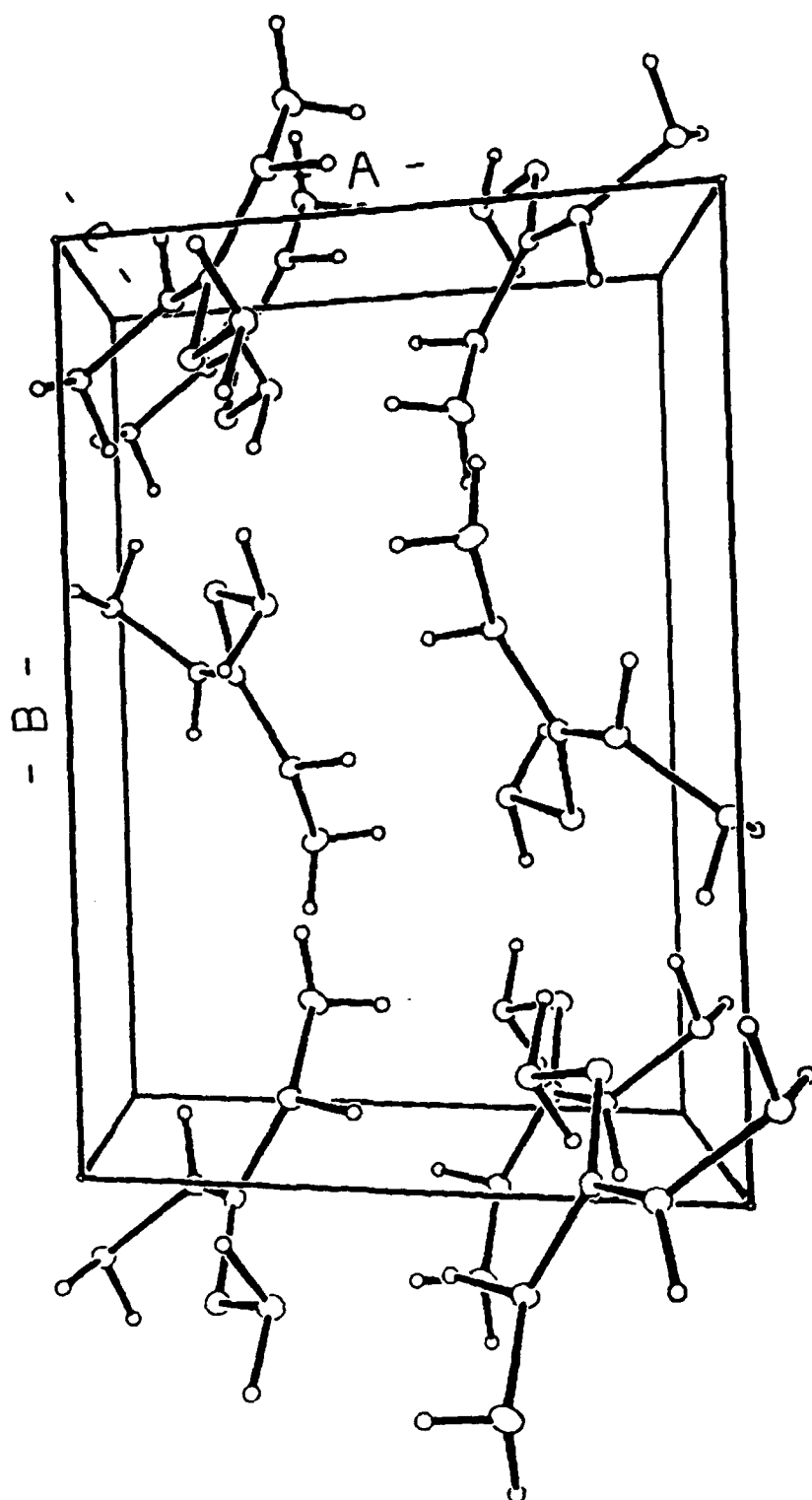


Figure 1. Unit cell of triaminoguanidine structure as viewed down the c axis. ORTEP plot with thermal ellipsoids scaled to enclose 20% probability (ref 12).

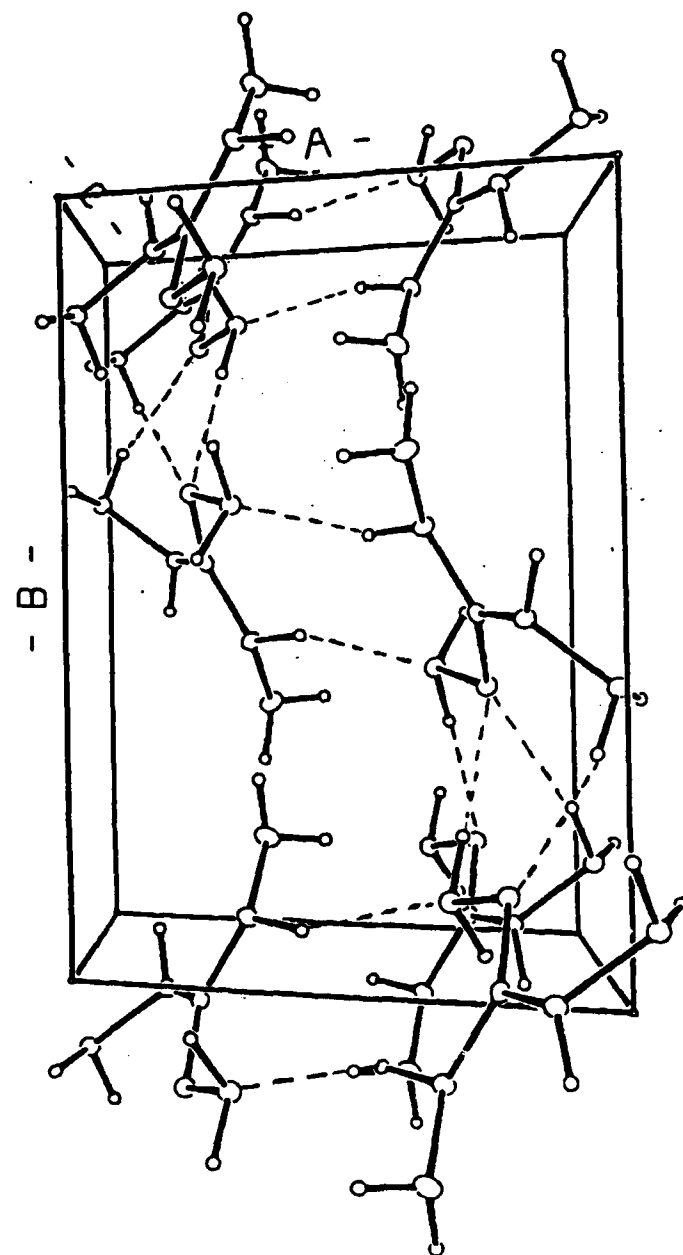


Figure 2. Unit cell of triaminoguanidine structure with hydrogen bonds viewed down the c axis.
ORTEP plot with thermal ellipsoids scaled to enclose 20% probability

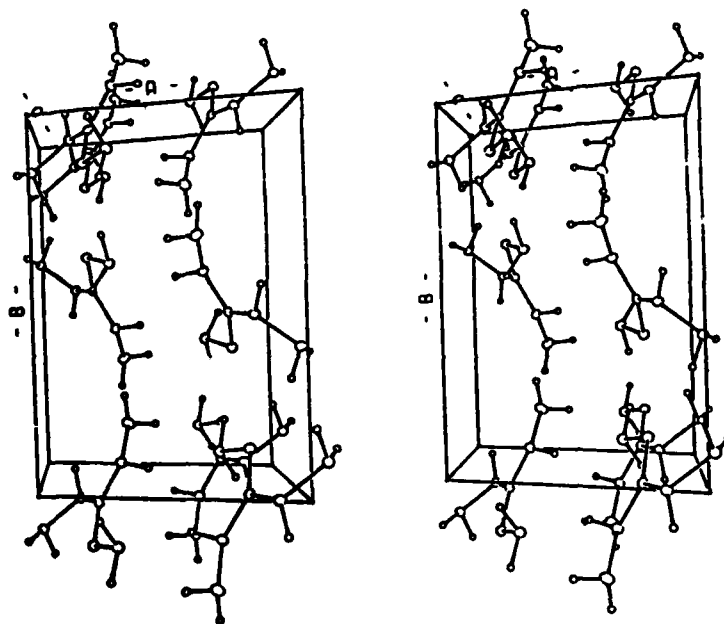


Figure 3. Stereographic pair of unit cells containing triaminoguanidine structure viewed down the c axis. ORTEP plot with thermal ellipsoids scaled to enclose 20% probability.

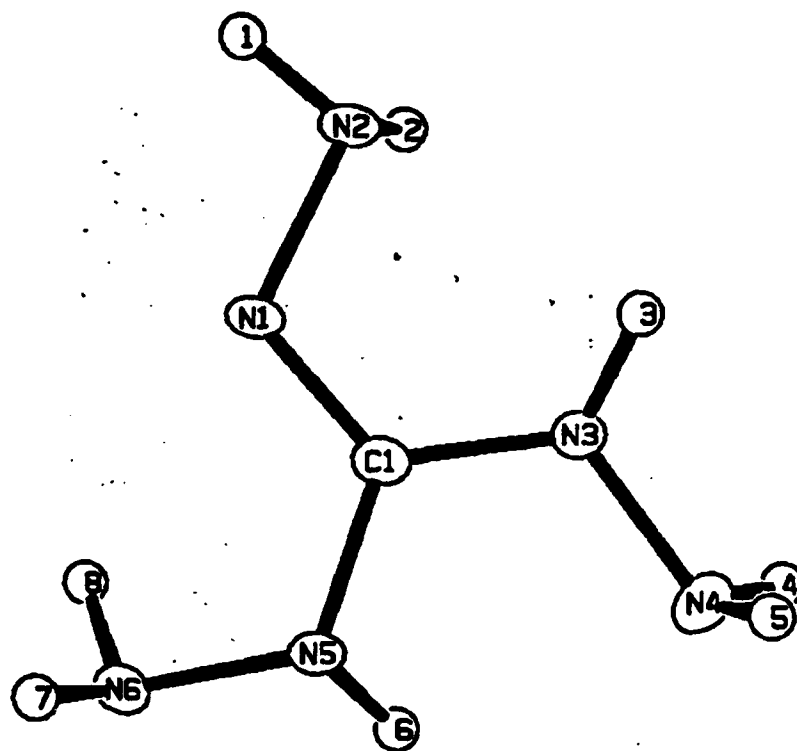


Figure 4. Triaminoguanidine molecule. ORTEP plot with thermal ellipsoids scaled to enclose 50% probability

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